

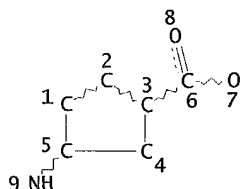
9 → 10

SOLOLA 10/019,217

=> d que 135
L13

STR

parent STR for all STRs



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

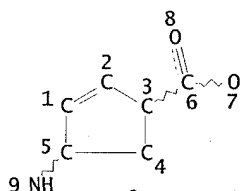
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

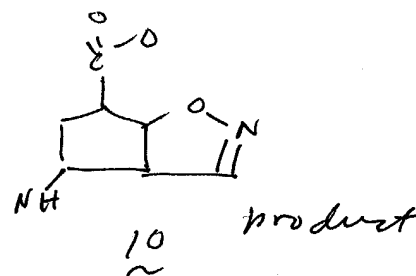
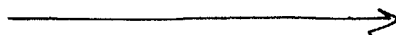
L15 1511 SEA FILE=REGISTRY SSS FUL L13

L16 18 SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND NOC3-C5/ES

L17 STR



reactant



product

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 1

CONNECT IS E2 RC AT 2

CONNECT IS E2 RC AT 4

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L19 85 SEA FILE=REGISTRY SUB=L15 SSS FUL L17

L31 88 SEA FILE=CAPLUS ABB=ON PLU=ON L19

L32 62 SEA FILE=CAPLUS ABB=ON PLU=ON L31(L)(RCT OR RACT)/RL ← reactant role

L34 5 SEA FILE=CAPLUS ABB=ON PLU=ON L16(L)PREP/RL ← product role

L35 5 SEA FILE=CAPLUS ABB=ON PLU=ON L32 AND L34 5 cites

=> d ibib abs hitstr 135 1-5

L35 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:314926 CAPLUS

DOCUMENT NUMBER: 136:325536

TITLE: Process for preparation of 4-N-substituted amino-2-aza-1-oxabicyclo[3.3.0]oct-2-ene-6-carboxylic acid esters and process for preparation of their intermediates

INVENTOR(S): Fukumoto, Takashi; Torihara, Masahiro; Tamai, Yoshin

PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

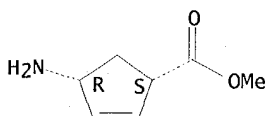
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002032885	A1	20020425	WO 2001-JP8627	20011001
W: US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
JP 2002193901	A2	20020710	JP 2001-281299	20010917
JP 2002234878	A2	20020823	JP 2001-281300	20010917
JP 2002284748	A2	20021003	JP 2001-281301	20010917
EP 1334969	A1	20030813	EP 2001-970314	20011001
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

PRIORITY APPLN. INFO.:
 JP 2000-317718 A 20001018
 JP 2000-369723 A 20001205
 JP 2001-7210 A 20010116
 WO 2001-JP8627 W 20011001

OTHER SOURCE(S): CASREACT 136:325536; MARPAT 136:325536
 AB 4-N-Substituted amino-2-aza-1-oxabicyclo[3.3.0]oct-2-ene-6-carboxylic acid esters, useful as pharmaceutical intermediates, are prepd. : (a) by reacting 2-azabicyclo[2.2.1]hept-5-en-3-one with an alc. in the presence of a Brønsted acid to form a salt of cis-4-amino-2-cyclopentene-1-carboxylic acid ester, (b) reacting this salt with a compd. for introducing an amino-protecting group in the presence of a base to form a cis-4-N-substituted amino-2-cyclopentene-1-carboxylic acid ester, (c) and reacting this ester with a hypohalite and an aldoxime.

IT 77745-25-6P 168683-02-1P 229613-91-6P
 414863-70-0P
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (process for prepn. of 4-N-substituted amino-2-aza-1-oxabicyclo[3.3.0]oct-2-ene-6-carboxylic acid esters and process for prepn. of their intermediates)
 RN 77745-25-6 CAPLUS
 CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, methyl ester, hydrochloride, (1R,4S)-rel- (9CI) (CA INDEX NAME)

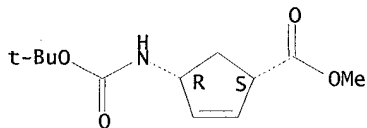
Relative stereochemistry.



● HCl

RN 168683-02-1 CAPLUS
 CN 2-Cyclopentene-1-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

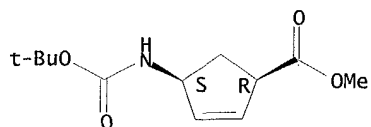


RN 229613-91-6 CAPLUS

SOLOLA 10/019,217

CN 2-Cyclopentene-1-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 414863-70-0 CAPLUS

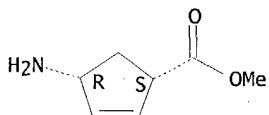
CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, methyl ester, cis-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 152279-17-9

CMF C7 H11 N O2

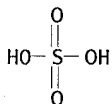
Relative stereochemistry.



CM 2

CRN 7664-93-9

CMF H2 O4 S



IT 229613-93-8P 229613-98-3P

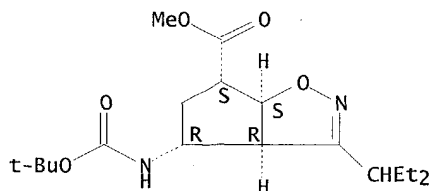
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(process for prepn. of 4-N-substituted amino-2-aza-1-oxabicyclo[3.3.0]oct-2-ene-6-carboxylic acid esters and process for prepn. of their intermediates)

RN 229613-93-8 CAPLUS

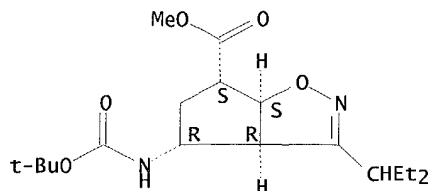
CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



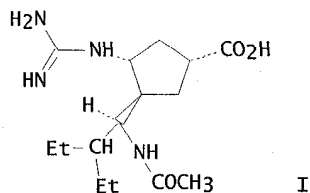
RN 229613-98-3 CAPLUS
 CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)-re1- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2001:787187 CAPLUS
 DOCUMENT NUMBER: 136:69605
 TITLE: Systematic Structure-Based Design and Stereoselective Synthesis of Novel Multi-Substituted Cyclopentane Derivatives with Potent Anti-influenza Activity
 AUTHOR(S): Chand, Pooran; Kotian, Pravin L.; Dehghani, Ali; El-Kattan, Yahya; Lin, Tsu-Hsing; Hutchison, Tracy L.; Babu, Y. Sudhakar; Bantia, Shanta; Elliott, Arthur J.; Montgomery, John A.
 CORPORATE SOURCE: BioCryst Pharmaceuticals Inc., Birmingham, AL, 35244, USA
 SOURCE: Journal of Medicinal Chemistry (2001), 44(25), 4379-4392
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The design and synthesis of novel, orally active, potent, and selective inhibitors of influenza neuraminidase differing structurally from existing neuraminidase inhibitors are described. X-ray crystal structures of complexes of neuraminidase with known five- and six-membered ring inhibitors revealed that potent inhibition of the enzyme is detd. by the relative positions of the interacting inhibitor substituents (carboxylate, glycerol, acetamido, hydroxyl) rather than by the abs. position of the central ring. This led us to design potential neuraminidase inhibitors in which the cyclopentane ring served as a scaffold for substituents (carboxylate, guanidino, acetamido, alkyl) that would interact with the four binding pockets of the neuraminidase active site at least as effectively as those of the established six-membered ring inhibitors such as DANA, zanamivir, and oseltamivir. A mixt. of the isomers was prepd. initially. Protein crystallog. of inhibitor-enzyme complexes was used to screen mixts. of isomers in order to identify the most active

stereoisomer. A synthetic route to the identified candidate cyclopentane I was developed, which featured (3+2) cycloaddn. of 2-ethylbutyronitrile oxide to Me (1S,4R)-4[(tert-butoxycarbonyl)amino]cyclopent-2-ene-1-carboxylate. Structures of the synthetic compds. were verified by NMR spectroscopy using nuclear Overhauser effect methodol. No new neuraminidase inhibitors discovered in this work, I has IC50 values vs neuraminidase from influenza A and B of <1 nM. These IC50 values are comparable or superior to those for zanamivir and oseltamivir, agents recently approved by the FDA for treatment of influenza.

IT 168683-02-1P 229613-83-6P 229613-93-8P

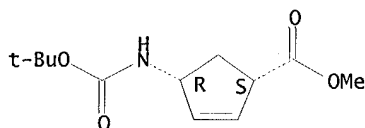
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(systematic structure-based design and stereoselective synthesis of novel multi-substituted cyclopentane derivs. with potent anti-influenza activity)

RN 168683-02-1 CAPLUS

CN 2-Cyclopentene-1-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1S,4R)- (9CI) (CA INDEX NAME)

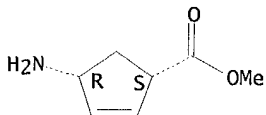
Absolute stereochemistry. Rotation (-).



RN 229613-83-6 CAPLUS

CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, methyl ester, hydrochloride, (1S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

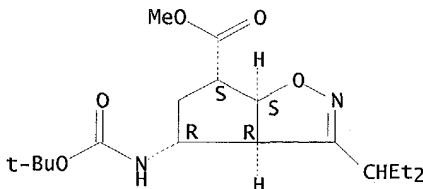


● HCl

RN 229613-93-8 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 383910-22-3P 383910-24-5P 383910-25-6P

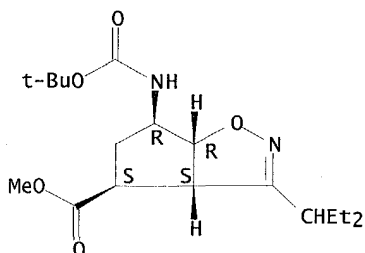
RL: SPN (Synthetic preparation); PREP (Preparation)

(systematic structure-based design and stereoselective synthesis of novel multi-substituted cyclopentane derivs. with potent anti-influenza activity)

RN 383910-22-3 CAPLUS

CN 4H-Cyclopent[d]isoxazole-4-carboxylic acid, 6-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aS,4S,6R,6aR)- (9CI) (CA INDEX NAME)

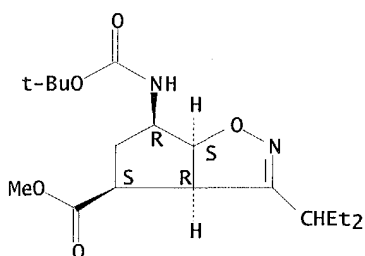
Absolute stereochemistry. Rotation (-).



RN 383910-24-5 CAPLUS

CN 4H-Cyclopent[d]isoxazole-4-carboxylic acid, 6-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4S,6R,6aS)- (9CI) (CA INDEX NAME)

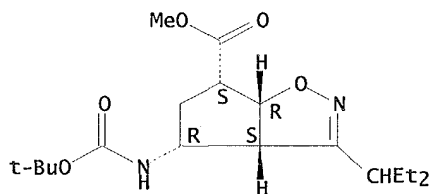
Absolute stereochemistry. Rotation (+).



RN 383910-25-6 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aS,4R,6S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:12411 CAPLUS

DOCUMENT NUMBER: 134:71317

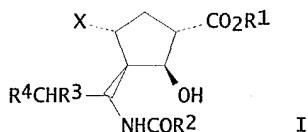
TITLE: Process for preparing substituted cyclopentane derivatives and their crystalline structures

INVENTOR(S): Abdel-Magid, Ahmed F.; Bichsel, Hans-Ulrich; Korey, Daniel J.; Laufer, Guenther G.; Lehto, Erja A.;

SOLOLA 10/019,217

PATENT ASSIGNEE(S): Mattei, Sebastiano; Rey, Max; Schultz, Thomas W.;
SOURCE: Maryanoff, Cynthia
Ortho-McNeil Pharmaceutical, Inc., USA
PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000571	A1	20010104	WO 2000-US16013	20000609
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000011902	A	20020319	BR 2000-11902	20000609
EP 1214294	A1	20020619	EP 2000-942747	20000609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003503384	T2	20030128	JP 2001-506983	20000609
US 2002061930	A1	20020523	US 2001-991753	20011126
US 6576786	B2	20030610		
NO 2001006389	A	20020221	NO 2001-6389	20011227
PRIORITY APPLN. INFO.: US 1999-141301P P 19990628				
US 2000-590839 A1 20000609				
WO 2000-US16013 W 20000609				
OTHER SOURCE(S): CASREACT 134:71317; MARPAT 134:71317				
GI				



AB Substituted cyclopentane derivs. I [R1 = H, alkyl, cycloalkyl, aryl, aralkyl; R2 = H, alkyl, haloalkyl, aryl, cycloalkyl; R3, R4 = H, alkyl, alkylene, cycloalkyl, aryl; X = NHC(:NH)NH2] were prepd. E.g., (1S,2S,3R,4R,1'S)-(-)-3-[(1'-acetylamino-2'-ethyl)butyl]-4-[[[aminoimino)methyl]amino]-2-hydroxycyclopentane-1-carboxylic acid was prepd.

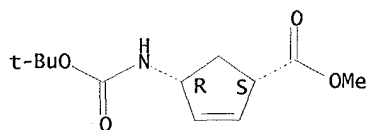
IT 168683-02-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of substituted cyclopentane derivs.)

RN 168683-02-1 CAPLUS

CN 2-Cyclopentene-1-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



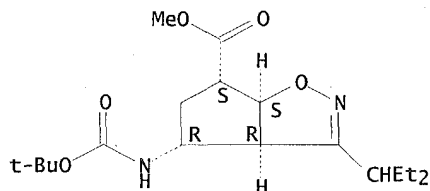
IT 229613-93-8P 316173-28-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of substituted cyclopentane derivs.)

RN 229613-93-8 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 316173-28-1 CAPLUS

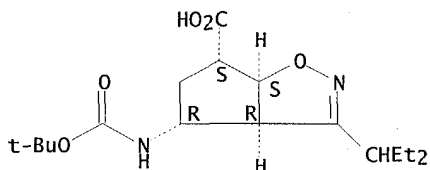
CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, (3aR,4R,6S,6aS)-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 316173-27-0

CMF C17 H28 N2 O5

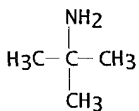
Absolute stereochemistry.



CM 2

CRN 75-64-9

CMF C4 H11 N



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:12400 CAPLUS

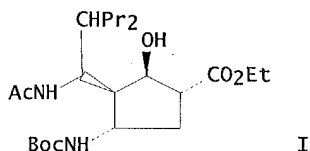
DOCUMENT NUMBER: 134:85973

TITLE: Preparation of substituted cyclopentane and cyclopentene compounds and certain intermediates

INVENTOR(S): Chand, Pooran; Elliott, Arthur J.

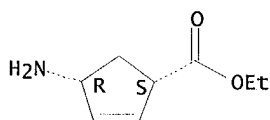
PATENT ASSIGNEE(S): Biocryst Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 53 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000558	A1	20010104	WO 2000-US17685	20000628
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG EP 1189862 A1 20020327 EP 2000-946871 20000628 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO PRIORITY APPLN. INFO.: US 1999-140840P P 19990628 WO 2000-US17685 W 20000628 OTHER SOURCE(S): MARPAT 134:85973 GI				



- AB Cyclopentanes such as I were prepd. from cyclopentane-fused isoxazolines, which were obtained by reaction of nitrile oxides with cyclopentenenes. Thus, a mixt. of 15 g Et c-4-[(tert-butoxycarbonyl)amino]-t-3-(2-propylbutyl)-4,5,6,6a-tetrahydro-2aH-cyclopent[d]isoxazole-6-r-carboxylate (II) in 120 mL EtOH/water/HOAc (1:1:1) contg. 1.5 g PtO2 was hydrogenated at 45 psi for 60 h to give 19 g (-)-t-3-(1-amino-2-propylpentyl)-c-4-[(tert-butoxycarbonyl)amino]-t-2-hydroxycyclopentane-r-1-carboxylate, which was acetylated by Ac2O in CH2Cl2 to give a 61% yield of I. The prepn. of II from 1-nitro-2-propylpentane, (-)-Et 4-[(tert-butoxycarbonyl)amino]cyclopentene-1-carboxylate, and PhNCO was described. The products were intended as neuraminidase inhibitors.
- IT 229613-86-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (cyclopentanecarboxylate derivs. as neuraminidase inhibitors)
- RN 229613-86-9 CAPLUS
- CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, ethyl ester, hydrochloride, (1S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



● HCl

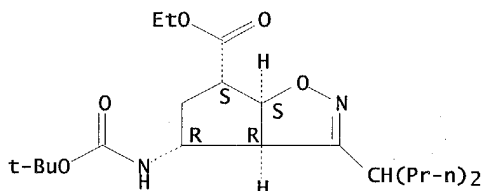
IT 316147-71-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cyclopentanecarboxylate derivs. as neuraminidase inhibitors)

RN 316147-71-4 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3a,5,6,6a-tetrahydro-3-(1-propylbutyl)-, ethyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:460384 CAPLUS

DOCUMENT NUMBER: 131:87678

TITLE: Preparation of substituted cyclopentane and cyclopentene compounds as neuraminidase inhibitors

INVENTOR(S): Babu, Yarlagadda S.; Chand, Pooran; Montgomery, John A.

PATENT ASSIGNEE(S): Biocryst Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 196 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

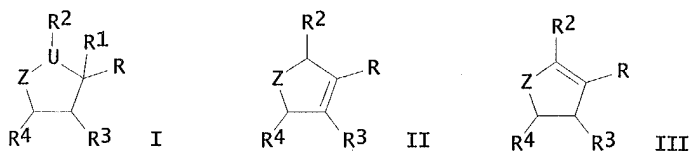
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WO 9933781	A1	19990708	WO 1998-US26871	19981217
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RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
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AU 9922001	A1	19990719	AU 1999-22001	19981217
ZA 9811595	A	20000619	ZA 1998-11595	19981217
EP 1040094	A1	20001004	EP 1998-966003	19981217

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

BR 9813480	A	20001010	BR 1998-13480	19981217
JP 2001527058	T2	20011225	JP 2000-526468	19981217
US 6562861	B1	20030513	US 2000-555131	20000525
NO 2000003084	A	20000814	NO 2000-3084	20000615

PRIORITY APPLN. INFO.: US 1997-69956P P 19971217
US 1998-85252P P 19980513
WO 1998-US26871 W 19981217

OTHER SOURCE(S): MARPAT 131:87678
GI



AB Title compds. I-III wherein U is CH, O, or S; Z is mono- or di-substituted carbon; R is (CH₂)_nCO₂H, (CH₂)_nSO₃H, (CH₂)_nPO₃H₂, (CH₂)_nNO₂, CH(SCH₃)₃, esters; R₁ is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl; R₂ is O; n is 0-4; R₃ is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl, haloalkyl; R₄ is (CH₂)_nOH, (CH₂)_nNH₂, substituted alkyl were prepd. as neuraminidase inhibitors. Thus, (1R,3R,4R,1'S)-(-)-(1'-acetylamino-2'-ethyl)butyl-4-(aminoimino)methylaminocyclopentan-1-carboxylic acid was prepd. and tested in vitro as neuraminidase inhibitor (IC₅₀ < 1 .mu.M).

IT 74201-87-9P 77745-25-6P 130931-84-9P
130931-85-0P 168683-02-1P 229613-83-6P
229613-86-9P 229613-87-0P 229613-88-1P
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229614-04-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of substituted cyclopentane and cyclopentene compds. as neuraminidase inhibitors)

RN 74201-87-9 CAPLUS

CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, hydrochloride, (1R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

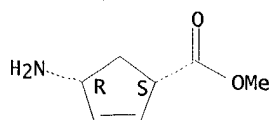


● HCl

RN 77745-25-6 CAPLUS

CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, methyl ester, hydrochloride, (1R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

RN 130931-84-9 CAPLUS
CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, hydrochloride, (1S,4R)- (9CI)
(CA INDEX NAME)

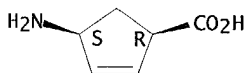
Absolute stereochemistry. Rotation (-).



● HCl

RN 130931-85-0 CAPLUS
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(CA INDEX NAME)

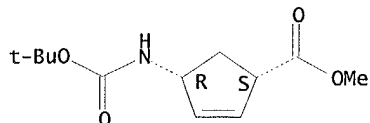
Absolute stereochemistry. Rotation (+).



● HCl

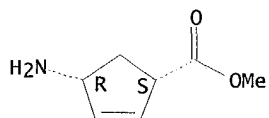
RN 168683-02-1 CAPLUS
CN 2-Cyclopentene-1-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-
methyl ester, (1S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 229613-83-6 CAPLUS
CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, methyl ester, hydrochloride,
(1S,4R)- (9CI) (CA INDEX NAME)

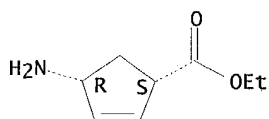
Absolute stereochemistry. Rotation (-).



● HCl

RN 229613-86-9 CAPLUS
CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, ethyl ester, hydrochloride,
(1S,4R)- (9CI) (CA INDEX NAME)

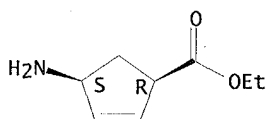
Absolute stereochemistry. Rotation (-).



● HCl

RN 229613-87-0 CAPLUS
CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, ethyl ester, hydrochloride,
(1R,4S)- (9CI) (CA INDEX NAME)

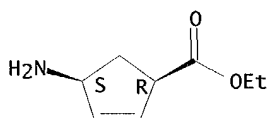
Absolute stereochemistry. Rotation (+).



● HCl

RN 229613-88-1 CAPLUS
CN 2-Cyclopentene-1-carboxylic acid, 4-amino-, ethyl ester, hydrochloride,
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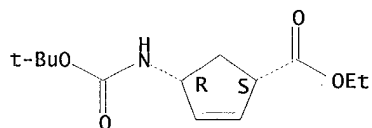
Relative stereochemistry.



● HCl

RN 229613-89-2 CAPLUS
CN 2-Cyclopentene-1-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-
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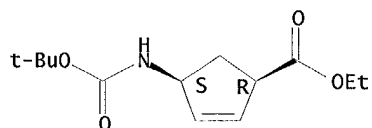
Absolute stereochemistry. Rotation (-).



RN 229613-90-5 CAPLUS

CN 2-Cyclopentene-1-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, ethyl ester, (1R,4S)- (9CI) (CA INDEX NAME)

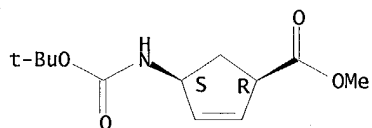
Absolute stereochemistry. Rotation (+).



RN 229613-91-6 CAPLUS

CN 2-Cyclopentene-1-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1R,4S)-rel- (9CI) (CA INDEX NAME)

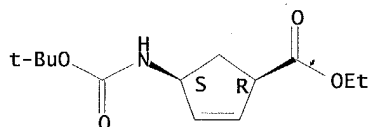
Relative stereochemistry.



RN 229613-92-7 CAPLUS

CN 2-Cyclopentene-1-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, ethyl ester, (1R,4S)-rel- (9CI) (CA INDEX NAME)

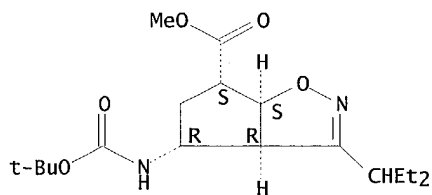
Relative stereochemistry.



RN 229613-93-8 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

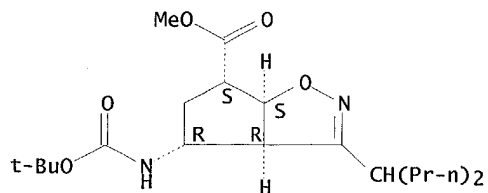


RN 229613-94-9 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-

dimethylethoxy)carbonyl]amino]-3a,5,6,6a-tetrahydro-3-(1-propylbutyl)-, methyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

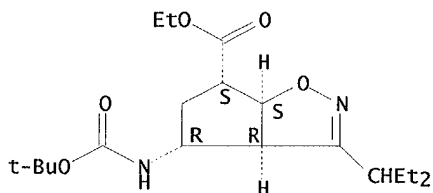
Absolute stereochemistry. Rotation (+).



RN 229613-95-0 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, ethyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

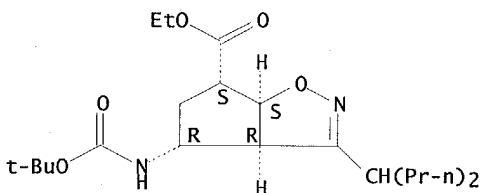
Absolute stereochemistry. Rotation (+).



RN 229613-96-1 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-propylbutyl)-, ethyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

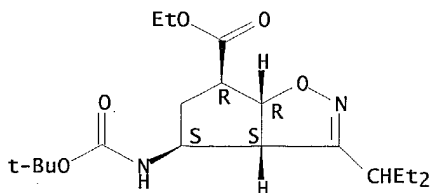
Absolute stereochemistry. Rotation (+).



RN 229613-97-2 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, ethyl ester, (3aS,4S,6R,6aR)- (9CI) (CA INDEX NAME)

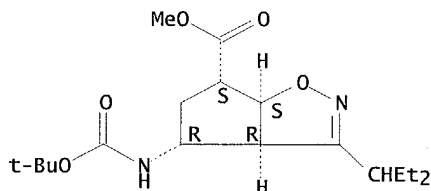
Absolute stereochemistry.



RN 229613-98-3 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

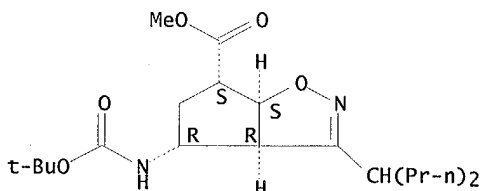
Relative stereochemistry.



RN 229613-99-4 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-propylbutyl)-, methyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

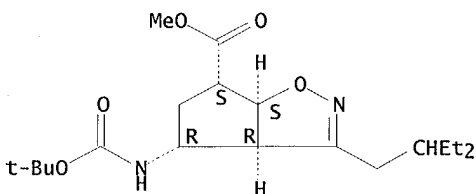
Relative stereochemistry.



RN 229614-00-0 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(2-ethylbutyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

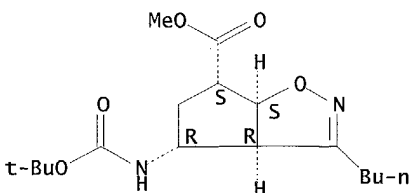
Relative stereochemistry.



RN 229614-01-1 CAPLUS

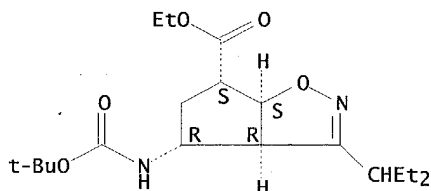
CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 3-butyl-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



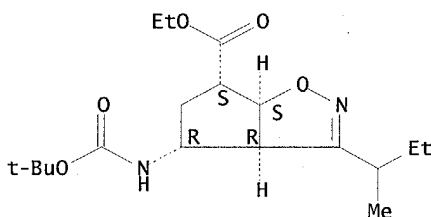
RN 229614-02-2 CAPLUS
 CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, ethyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



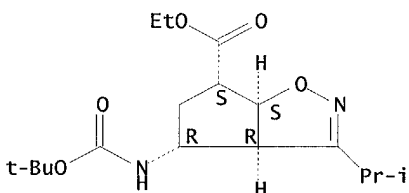
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 CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-methylpropyl)-, ethyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 229614-04-4 CAPLUS
 CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-methylethyl)-, ethyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

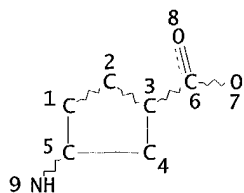
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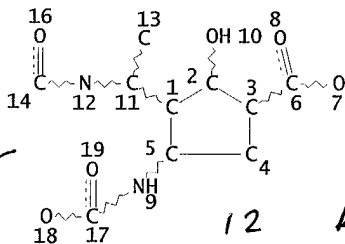
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
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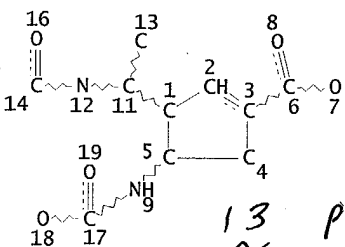


12 Reactant

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
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13 product

NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

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 L43 1 SEA FILE=CAPLUS ABB=ON PLU=ON L40 AND L41 1 citation

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L43 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:460384 CAPLUS

DOCUMENT NUMBER: 131:87678

TITLE: Preparation of substituted cyclopentane and cyclopentene compounds as neuraminidase inhibitors

INVENTOR(S): Babu, Yarlagadda S.; Chand, Pooran; Montgomery, John A.

PATENT ASSIGNEE(S): Biocryst Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 196 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

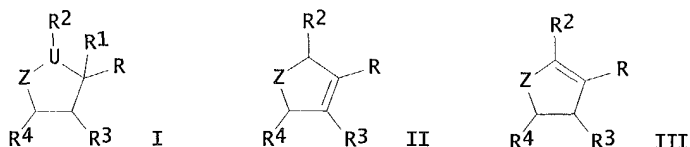
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933781	A1	19990708	WO 1998-US26871	19981217
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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EP 1040094	A1	20001004	EP 1998-966003	19981217
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PRIORITY APPLN. INFO.:			US 1997-69956P	P 19971217
			US 1998-85252P	P 19980513
			WO 1998-US26871	W 19981217

OTHER SOURCE(S): MARPAT 131:87678

GI



AB Title compds. I-III wherein U is CH, O, or S; Z is mono- or di-substituted carbon; R is (CH₂)_nCO₂H, (CH₂)_nSO₃H, (CH₂)_nPO₃H₂, (CH₂)_nNO₂, CH(SCH₃)₃, esters; R1 is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl; RR1 is O; n is 0-4; R2, R3 is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl, haloalkyl; R4 is (CH₂)_nOH, (CH₂)_nNH₂, substituted alkyl were prepd. as neuraminidase inhibitors. Thus, (1R,3R,4R,1'S)-(-)-(1'-acetylamino-2'-ethyl)butyl-4-

(aminoimino)methylaminocyclopentan-1-carboxylic acid was prepd. and tested in vitro as neuraminidase inhibitor (IC50 < 1 .mu.M).

IT 229614-05-5P 229614-06-6P 229614-07-7P

229614-08-8P 229614-09-9P 229614-10-2P

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP

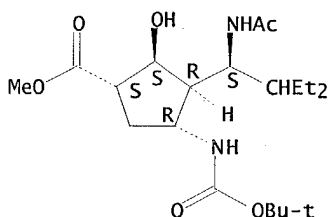
(Preparation); RACT (Reactant or reagent)

(prepn. of substituted cyclopentane and cyclopentene compds. as neuraminidase inhibitors)

RN 229614-05-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetyl amino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

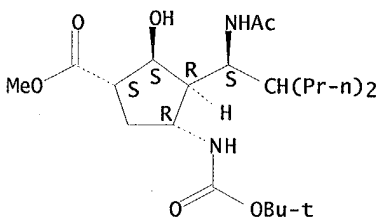
Absolute stereochemistry. Rotation (-).



RN 229614-06-6 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetyl amino)-2-propylpentyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

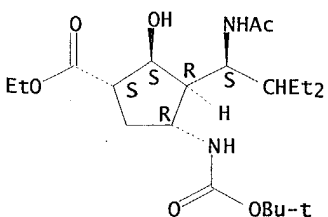
Absolute stereochemistry. Rotation (-).



RN 229614-07-7 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetyl amino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

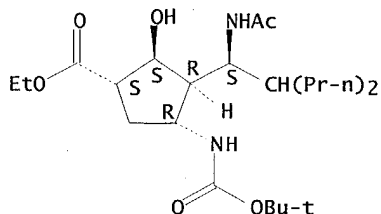


RN 229614-08-8 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetyl amino)-2-propylpentyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

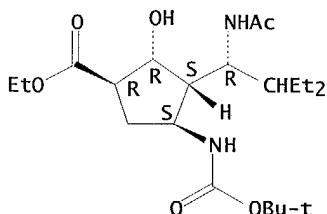
Absolute stereochemistry. Rotation (-).



RN 229614-09-9 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy]carbonyl]amino]-2-hydroxy-, ethyl ester, (1R,2R,3S,4S)- (9CI) (CA INDEX NAME)

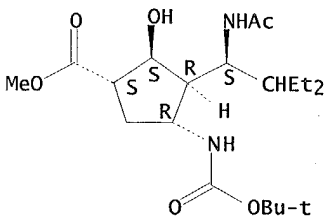
Absolute stereochemistry. Rotation (+).



RN 229614-10-2 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy]carbonyl]amino]-2-hydroxy-, methyl ester, (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

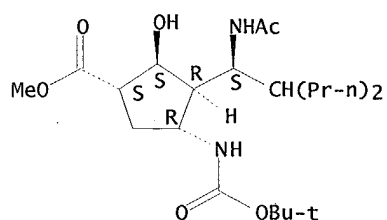


RN 229614-11-3 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-propylpentyl]-4-[[[1,1-dimethylethoxy]carbonyl]amino]-2-hydroxy-, methyl ester, (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

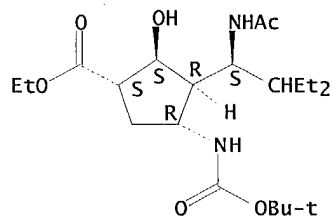
SOLOLA 10/019,217



RN 229614-14-6 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

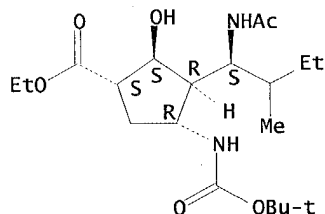
Relative stereochemistry.



RN 229614-15-7 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-methylbutyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

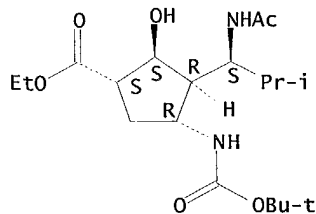
Relative stereochemistry.



RN 229614-16-8 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-methylpropyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

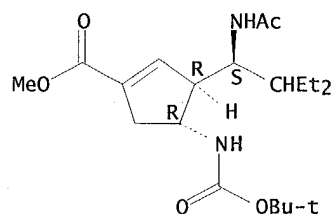


RN 229614-98-6 CAPLUS

SOLOLA 10/019,217

CN 1-Cyclopentene-1-carboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (3R,4R)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



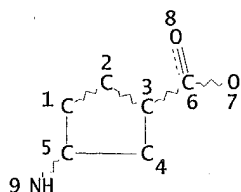
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

16 → 12
~ ~

SOLOLA 10/019,217

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L13

STR parent str

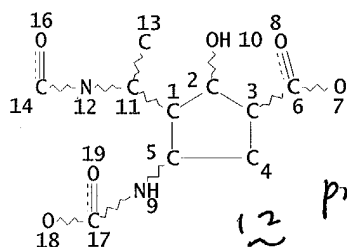


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

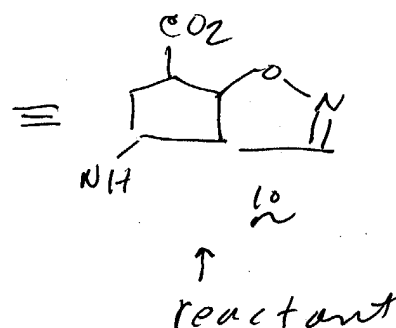
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L15 1511 SEA FILE=REGISTRY SSS FUL L13
L16 18 SEA FILE=REGISTRY ABB=ON PLU=ON L15 AND NOC3-C5/ES
L21 STR



product



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L23 22 SEA FILE=REGISTRY SUB=L15 SSS FUL L21
L36 3 SEA FILE=CAPLUS ABB=ON PLU=ON L16(L)(RCT OR RACT)/RL 10 as reactant
L37 5 SEA FILE=CAPLUS ABB=ON PLU=ON L23
L38 5 SEA FILE=CAPLUS ABB=ON PLU=ON L37(L)PREP/RL 12 as product
L39 3 SEA FILE=CAPLUS ABB=ON PLU=ON L36 AND L38 3 cites

=> d ibib abs hitstr 139 1-3

L39 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:787187 CAPLUS

DOCUMENT NUMBER: 136:69605

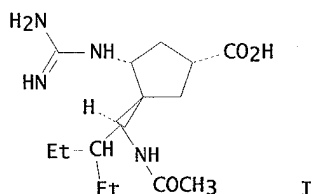
TITLE: Systematic Structure-Based Design and Stereoselective
Synthesis of Novel Multi-Substituted Cyclopentane
Derivatives with Potent Anti-influenza Activity
AUTHOR(S): Chand, Pooran; Kotian, Pravin L.; Dehghani, Ali;
El-Kattan, Yahya; Lin, Tsu-Hsing; Hutchison, Tracy L.;
Babu, Y. Sudhakar; Bantia, Shanta; Elliott, Arthur J.;
Montgomery, John A.

CORPORATE SOURCE: BioCryst Pharmaceuticals Inc., Birmingham, AL, 35244,
USA

SOURCE: Journal of Medicinal Chemistry (2001), 44(25),

4379-4392
 CODEN: JMCMAR; ISSN: 0022-2623
 American Chemical Society
 Journal
 English

PUBLISHER:
 DOCUMENT TYPE:
 LANGUAGE:
 GI

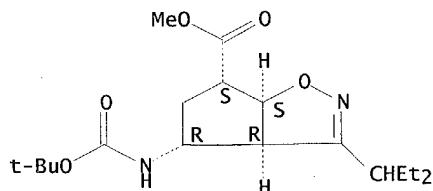


AB The design and synthesis of novel, orally active, potent, and selective inhibitors of influenza neuraminidase differing structurally from existing neuraminidase inhibitors are described. X-ray crystal structures of complexes of neuraminidase with known five- and six-membered ring inhibitors revealed that potent inhibition of the enzyme is detd. by the relative positions of the interacting inhibitor substituents (carboxylate, glycerol, acetamido, hydroxyl) rather than by the abs. position of the central ring. This led us to design potential neuraminidase inhibitors in which the cyclopentane ring served as a scaffold for substituents (carboxylate, guanidino, acetamido, alkyl) that would interact with the four binding pockets of the neuraminidase active site at least as effectively as those of the established six-membered ring inhibitors such as DANA, zanamivir, and oseltamivir. A mixt. of the isomers was prepd. initially. Protein crystallog. of inhibitor-enzyme complexes was used to screen mixts. of isomers in order to identify the most active stereoisomer. A synthetic route to the identified candidate cyclopentane I was developed, which featured (3+2) cycloaddn. of 2-ethylbutyronitrile oxide to Me (1S,4R)-4[(tert-butoxycarbonyl)amino]cyclopent-2-ene-1-carboxylate. Structures of the synthetic compds. were verified by NMR spectroscopy using nuclear Overhauser effect methodol. No new neuraminidase inhibitors discovered in this work, I has IC50 values vs neuraminidase from influenza A and B of <1 nM. These IC50 values are comparable or superior to those for zanamivir and oseltamivir, agents recently approved by the FDA for treatment of influenza.

IT 229613-93-8P 229614-05-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (systematic structure-based design and stereoselective synthesis of novel multi-substituted cyclopentane derivs. with potent anti-influenza activity)

RN 229613-93-8 CAPLUS
 CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

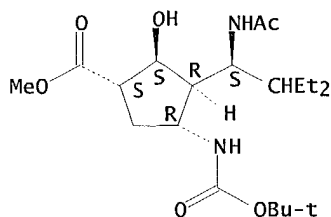


RN 229614-05-5 CAPLUS

SOLOLA 10/019,217

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:12411 CAPLUS

DOCUMENT NUMBER: 134:71317

TITLE: Process for preparing substituted cyclopentane
derivatives and their crystalline structures

INVENTOR(S): Abdel-Magid, Ahmed F.; Bichsel, Hans-Ulrich; Korey,
Daniel J.; Laufer, Guenther G.; Lehto, Erja A.;
Mattei, Sebastiano; Rey, Max; Schultz, Thomas W.;
Maryanoff, Cynthia

PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA

SOURCE: PCT Int. Appl., 68 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

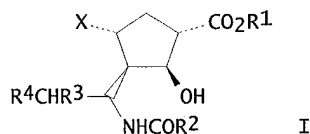
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000571	A1	20010104	WO 2000-US16013	20000609
W:				
AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,				
CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,				
ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,				
LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,				
SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA,				
ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW:				
GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,				
CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000011902	A	20020319	BR 2000-11902	20000609
EP 1214294	A1	20020619	EP 2000-942747	20000609
R:				
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003503384	T2	20030128	JP 2001-506983	20000609
US 2002061930	A1	20020523	US 2001-991753	20011126
US 6576786	B2	20030610		
NO 2001006389	A	20020221	NO 2001-6389	20011227

PRIORITY APPLN. INFO.:

US 1999-141301P P 19990628
US 2000-590839 A1 20000609
WO 2000-US16013 W 20000609

OTHER SOURCE(S): CASREACT 134:71317; MARPAT 134:71317

GI



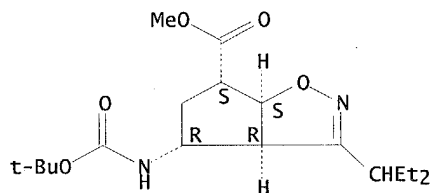
AB Substituted cyclopentane derivs. I [R1 = H, alkyl, cycloalkyl, aryl, aralkyl; R2 = H, alkyl, haloalkyl, aryl, cycloalkyl; R3, R4 = H, alkyl, alkylene, cycloalkyl, aryl; X = NHC(:NH)NH2] were prepd. E.g., (1S,2S,3R,4R,1'S)-(-)-3-[(1'-acetylamino-2'-ethyl)butyl]-4-[[[aminoimino)methyl]amino]-2-hydroxycyclopentane-1-carboxylic acid was prepd.

IT 229613-93-8P 316173-28-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of substituted cyclopentane derivs.)

RN 229613-93-8 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 316173-28-1 CAPLUS

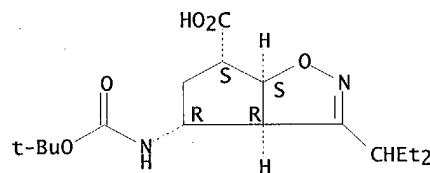
CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, (3aR,4R,6S,6aS)-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 316173-27-0

CMF C17 H28 N2 O5

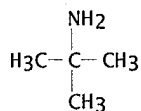
Absolute stereochemistry.



CM 2

CRN 75-64-9

CMF C4 H11 N



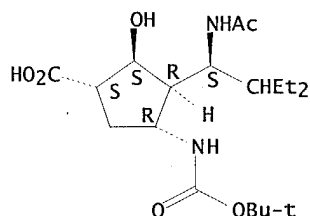
IT 316173-30-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of substituted cyclopentane derivs.)

RN 316173-30-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, (1S,2S,3R,4R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:460384 CAPLUS

DOCUMENT NUMBER: 131:87678

TITLE: Preparation of substituted cyclopentane and cyclopentene compounds as neuraminidase inhibitors

INVENTOR(S): Babu, Yarlagadda S.; Chand, Pooran; Montgomery, John A.

PATENT ASSIGNEE(S): Biocryst Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 196 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

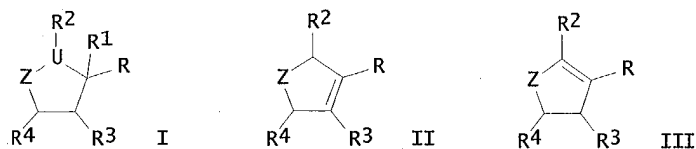
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933781	A1	19990708	WO 1998-US26871	19981217
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2315262	AA	19990708	CA 1998-2315262	19981217
AU 9922001	A1	19990719	AU 1999-22001	19981217
ZA 9811595	A	20000619	ZA 1998-11595	19981217
EP 1040094	A1	20001004	EP 1998-966003	19981217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9813480	A	20001010	BR 1998-13480	19981217
JP 2001527058	T2	20011225	JP 2000-526468	19981217

SOLOLA 10/019,217

US 6562861 B1 20030513 US 2000-555131 20000525
NO 2000003084 A 20000814 NO 2000-3084 20000615
PRIORITY APPLN. INFO.: US 1997-69956P P 19971217
US 1998-85252P P 19980513
WO 1998-US26871 W 19981217

OTHER SOURCE(S): MARPAT 131:87678
GI



AB Title compds. I-III wherein U is CH, O, or S; Z is mono- or di-substituted carbon; R is (CH₂)_nCO₂H, (CH₂)_nSO₃H, (CH₂)_nPO₃H₂, (CH₂)_nNO₂, CH(SCH₃)₃, esters; R₁ is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl; R₂ is O; n is 0-4; R₃ is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl, haloalkyl; R₄ is (CH₂)_nOH, (CH₂)_nNH₂, substituted alkyl were prepd. as neuraminidase inhibitors. Thus, (1R,3R,4R,1'S)-(-)-(1'-acetylamino-2'-ethyl)butyl-4-(aminoimino)methylaminocyclopentan-1-carboxylic acid was prepd. and tested in vitro as neuraminidase inhibitor (IC₅₀ < 1 .mu.M).

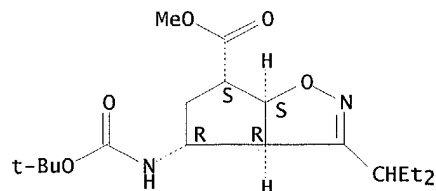
IT 229613-93-8P 229613-94-9P 229613-95-0P
229613-96-1P 229613-97-2P 229613-98-3P
229613-99-4P 229614-00-0P 229614-01-1P
229614-02-2P 229614-03-3P 229614-04-4P
229614-05-5P 229614-06-6P 229614-07-7P
229614-08-8P 229614-09-9P 229614-10-2P
229614-11-3P 229614-14-6P 229614-15-7P
229614-16-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of substituted cyclopentane and cyclopentene compds. as neuraminidase inhibitors)

RN 229613-93-8 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)]-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

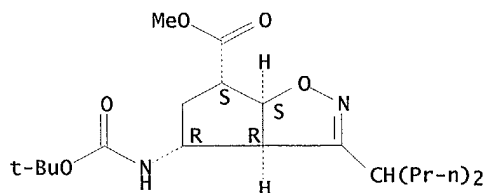
Absolute stereochemistry. Rotation (+).



RN 229613-94-9 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-propylbutyl)]-, methyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

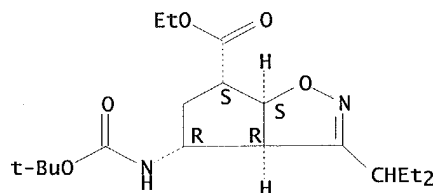
Absolute stereochemistry. Rotation (+).



RN 229613-95-0 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, ethyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

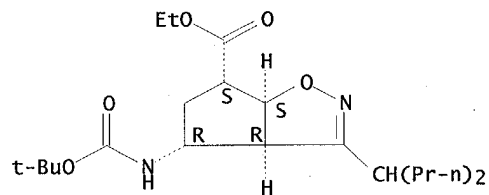
Absolute stereochemistry. Rotation (+).



RN 229613-96-1 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, ethyl ester, (3aR,4R,6S,6aS)- (9CI) (CA INDEX NAME)

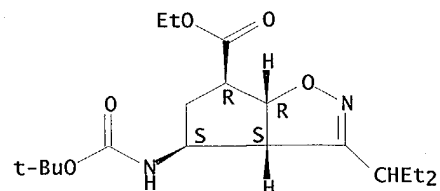
Absolute stereochemistry. Rotation (+).



RN 229613-97-2 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, ethyl ester, (3aS,4S,6R,6aR)- (9CI) (CA INDEX NAME)

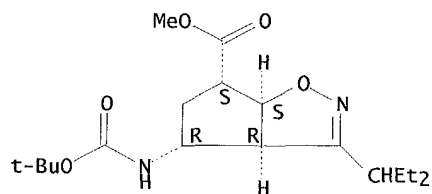
Absolute stereochemistry.



RN 229613-98-3 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

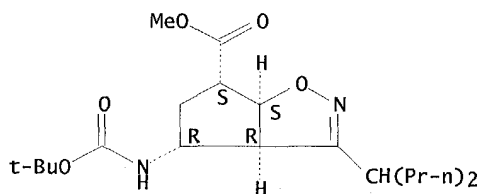
Relative stereochemistry.



RN 229613-99-4 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3a,5,6,6a-tetrahydro-3-(1-propylbutyl)-, methyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

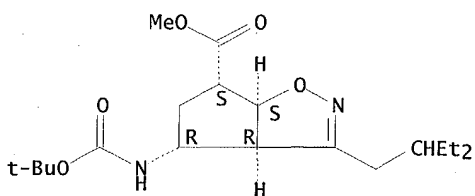
Relative stereochemistry.



RN 229614-00-0 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(2-ethylbutyl)-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

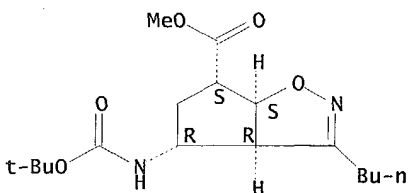
Relative stereochemistry.



RN 229614-01-1 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 3-butyl-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3a,5,6,6a-tetrahydro-, methyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

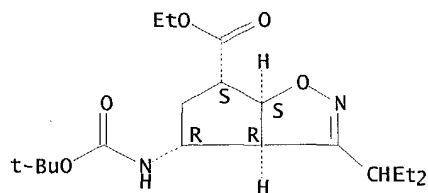
Relative stereochemistry.



RN 229614-02-2 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-ethylpropyl)-3a,5,6,6a-tetrahydro-, ethyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

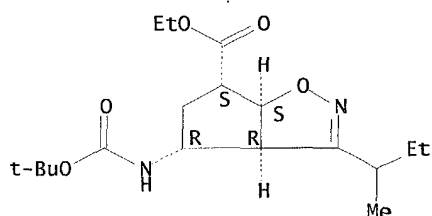
Relative stereochemistry.



RN 229614-03-3 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3a,5,6,6a-tetrahydro-3-(1-methylpropyl)-, ethyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

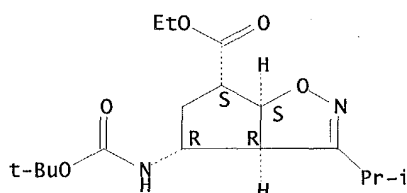
Relative stereochemistry.



RN 229614-04-4 CAPLUS

CN 4H-Cyclopent[d]isoxazole-6-carboxylic acid, 4-[[[(1,1-dimethylethoxy)carbonyl]amino]-3a,5,6,6a-tetrahydro-3-(1-methylethyl)-, ethyl ester, (3aR,4R,6S,6aS)-rel- (9CI) (CA INDEX NAME)

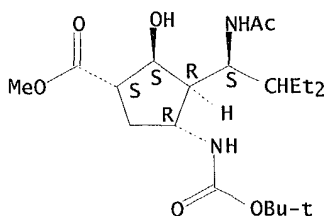
Relative stereochemistry.



RN 229614-05-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

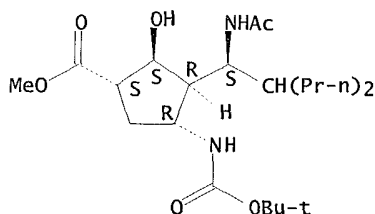
Absolute stereochemistry. Rotation (-).



RN 229614-06-6 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-propylpentyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

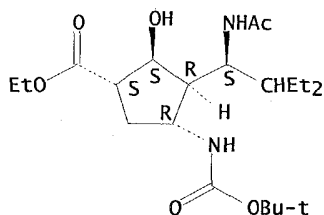
Absolute stereochemistry. Rotation (-).



RN 229614-07-7 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

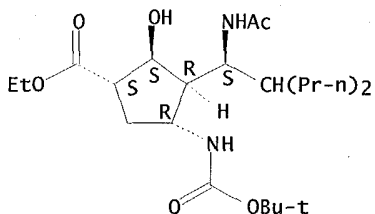
Absolute stereochemistry. Rotation (-).



RN 229614-08-8 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-propylpentyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

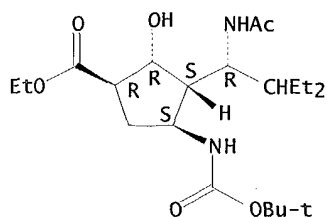
Absolute stereochemistry. Rotation (-).



RN 229614-09-9 CAPLUS

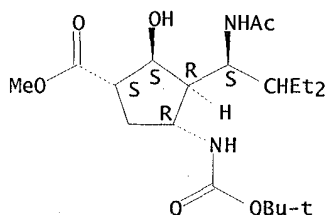
CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1R,2R,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



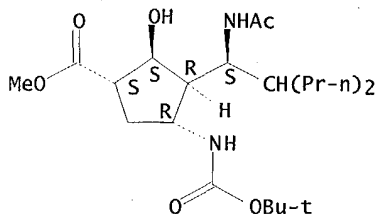
RN 229614-10-2 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy]carbonyl]amino]-2-hydroxy-, methyl ester, (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



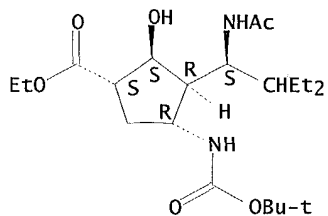
RN 229614-11-3 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-propylpentyl]-4-[[[1,1-dimethylethoxy]carbonyl]amino]-2-hydroxy-, methyl ester, (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 229614-14-6 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy]carbonyl]amino]-2-hydroxy-, ethyl ester, (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

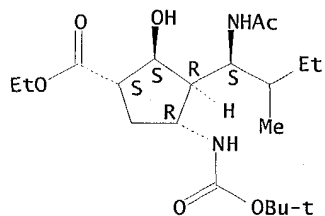


RN 229614-15-7 CAPLUS

SOLOLA 10/019,217

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-methylbutyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

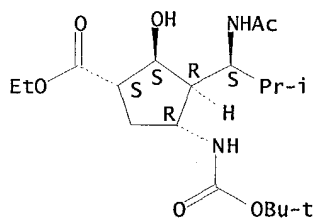
Relative stereochemistry.



RN 229614-16-8 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-methylpropyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

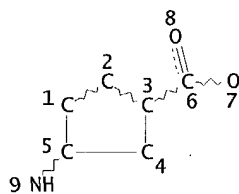
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THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d que 146
L13

STR

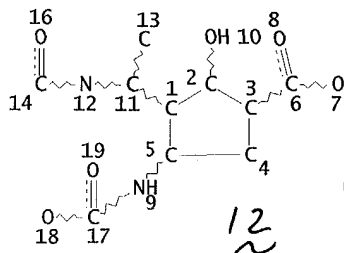
parent STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
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L21 STR

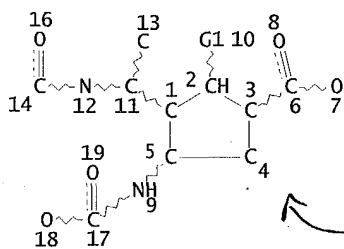


reactant

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L23 22 SEA FILE=REGISTRY SUB=L15 SSS FUL L21
L24 STR



product

converting OH group of 12 to F, OR, O-CR, NH or NH-CR

VAR G1=F/NH/20
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 20
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 19

p48 -49 of claims

STEREO ATTRIBUTES: NONE

L26 11 SEA FILE=REGISTRY SUB=L15 SSS FUL L24
 L40 3 SEA FILE=CAPLUS ABB=ON PLU=ON L23(L)(RCT OR RACT)/RL *12 as reactant*
 L45 4 SEA FILE=CAPLUS ABB=ON PLU=ON L26(L)PREP/RL
 L46 3 SEA FILE=CAPLUS ABB=ON PLU=ON L40 AND L45 *3 cites*

=> d ibib abs hitstr 146 1-3

L46 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:787187 CAPLUS

DOCUMENT NUMBER: 136:69605

TITLE: Systematic Structure-Based Design and Stereoselective Synthesis of Novel Multi-Substituted Cyclopentane Derivatives with Potent Anti-influenza Activity

AUTHOR(S): Chand, Pooran; Kotian, Pravin L.; Dehghani, Ali; El-Kattan, Yahya; Lin, Tsu-Hsing; Hutchison, Tracy L.; Babu, Y. Sudhakar; Bantia, Shanta; Elliott, Arthur J.; Montgomery, John A.

CORPORATE SOURCE: BioCryst Pharmaceuticals Inc., Birmingham, AL, 35244, USA

SOURCE: Journal of Medicinal Chemistry (2001), 44(25), 4379-4392

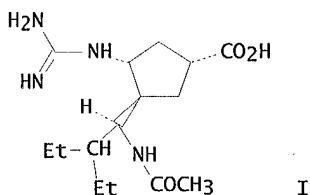
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The design and synthesis of novel, orally active, potent, and selective inhibitors of influenza neuraminidase differing structurally from existing neuraminidase inhibitors are described. X-ray crystal structures of complexes of neuraminidase with known five- and six-membered ring inhibitors revealed that potent inhibition of the enzyme is detd. by the relative positions of the interacting inhibitor substituents (carboxylate, glycerol, acetamido, hydroxyl) rather than by the abs. position of the central ring. This led us to design potential neuraminidase inhibitors in which the cyclopentane ring served as a scaffold for substituents (carboxylate, guanidino, acetamido, alkyl) that would interact with the four binding pockets of the neuraminidase active site at least as effectively as those of the established six-membered ring inhibitors such as DANA, zanamivir, and oseltamivir. A mixt. of the isomers was prepd. initially. Protein crystallog. of inhibitor-enzyme complexes was used to screen mixts. of isomers in order to identify the most active stereoisomer. A synthetic route to the identified candidate cyclopentane I was developed, which featured (3+2) cycloaddn. of 2-ethylbutyronitrile oxide to Me (1S,4R)-4[(tert-butoxycarbonyl)amino]cyclopent-2-ene-1-carboxylate. Structures of the synthetic compds. were verified by NMR spectroscopy using nuclear Overhauser effect methodol. No new neuraminidase inhibitors discovered in this work, I has IC50 values vs neuraminidase from influenza A and B of <1 nM. These IC50 values are comparable or superior to those for zanamivir and oseltamivir, agents recently approved by the FDA for treatment of influenza.

IT 229614-05-5P 229614-61-3P

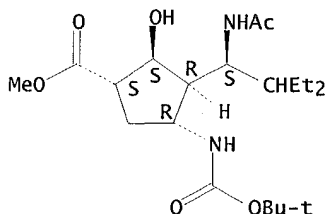
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(systematic structure-based design and stereoselective synthesis of novel multi-substituted cyclopentane derivs. with potent anti-influenza activity)

RN 229614-05-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

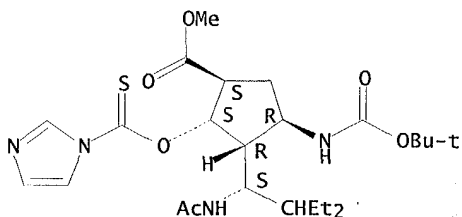
Absolute stereochemistry. Rotation (-).



RN 229614-61-3 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-(1H-imidazol-1-ylthioxomethoxy)-, methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:635885 CAPLUS

DOCUMENT NUMBER: 135:210771

TITLE: Preparation of prodrugs of substituted cyclopentane and cyclopentene compounds useful as neuraminidase inhibitors

INVENTOR(S): Babu, Yarlagadda S.; Chand, Pooran; Montgomery, John A.; Watts, Karen Bush; Hlasta, Dennis J.; Caldwell, Gary W.

PATENT ASSIGNEE(S): Biocryst Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 109 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062242	A1	20010830	WO 2001-US5862	20010226
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,				

SOLOLA 10/019,217

LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-184666P P 20000224

OTHER SOURCE(S): MARPAT 135:210771

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H, R5, (CH2)nOC(O)R5, (CH2)nOR5, (CH2)n-N-R6; R2-3 = H, (CH2)mOH, C(O)OR, C(O)R5, C(O)SR, (CH2)mC(O)NR5R5', OC(O)OR5, an amino acid and/or a dipeptide; R = R5, H, etc.; R4 = H, OH, OC(O)R5, OC(O)NR5R5', OC(O)OR5; R5-5' = H, alk(en/yn)yl, aryl, heterocycle, alkylaryl, cycloalkyl, CH2CO2alkyl; and wherein R5 can be (dialkyl)CO alkyl; R6 NR6 = phthalimido, etc.; R7-7' = alkyl, alkylaryl, cycloalkyl; R8 = (halo)alkyl; n = 1 - 5; m = 0 - 4] were prepd. Over 40 synthetic examples were prepd. For instance, reaction of II.bul.CF3CO2H and isothiurea III (prepn. given) (DMF, Et3N, HgCl2, 2 h) followed by hydrogenation (MeOHaq, HCl, H2/10% Pd-C @ 40 psi, 16 h) provided IV (68% yield, 2 steps). The synthesis of II (and derivs.) is claimed (II was disclosed in prior art). Compds. I are prodrugs that inhibit influenza virus neuraminidase (no data) and may be used for preventing, treating or ameliorating viral and bacterial infections.

IT 316173-30-5P 357447-47-3P 357447-49-5P
357447-53-1P 357447-93-9P 357447-99-5P
357448-03-4P 357448-07-8P 357448-11-4P
357448-15-8P 357448-19-2P 357448-23-8P
357448-27-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

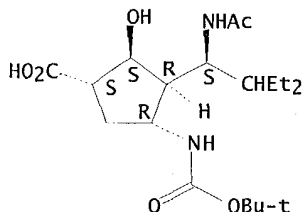
(Preparation); RACT (Reactant or reagent)

(intermediate; synthesis of guanidino-cyclopentyl-carboxy derivs.
(prodrugs) as neuraminidase inhibitors)

RN 316173-30-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, (1S,2S,3R,4R)- (9CI)
(CA INDEX NAME)

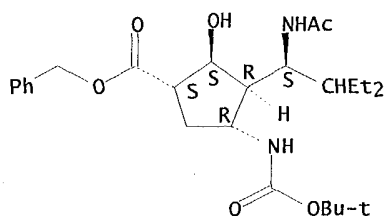
Absolute stereochemistry. Rotation (-).



RN 357447-47-3 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, phenylmethyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

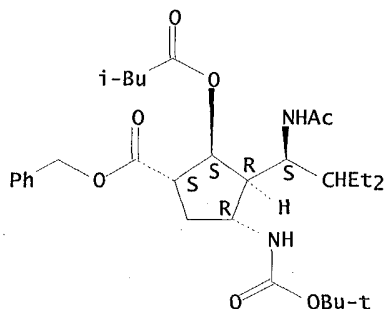
Absolute stereochemistry. Rotation (-).



RN 357447-49-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-(3-methyl-1-oxobutoxy)-, phenylmethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

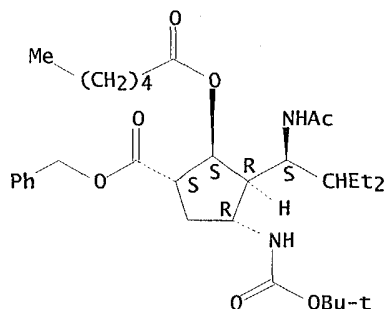
Absolute stereochemistry. Rotation (-).



RN 357447-53-1 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-[(1-oxohexyl)oxy]-, phenylmethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

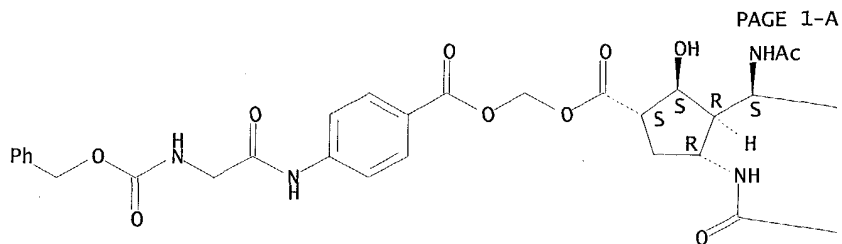
Absolute stereochemistry. Rotation (-).



RN 357447-93-9 CAPLUS

CN Benzoic acid, 4-[[[[(phenylmethoxy)carbonyl]amino]acetyl]amino]-, [[[(1S,2S,3R,4R)-3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxycyclopentyl]carbonyl]oxy]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



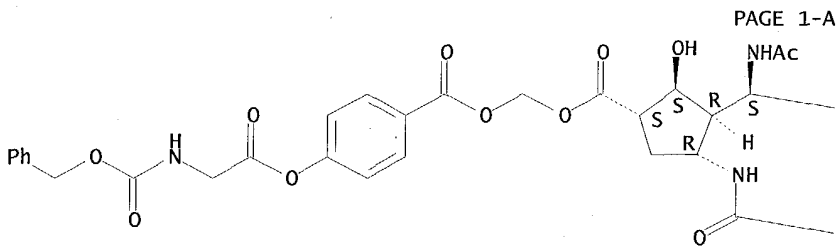
PAGE 1-B

CHET2

OBu-t

RN 357447-99-5 CAPLUS
 CN Glycine, N-[(phenylmethoxy)carbonyl]-, 4-[[[[(1S,2S,3R,4R)-3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxycyclopentyl]carbonyl]oxy]methoxy]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



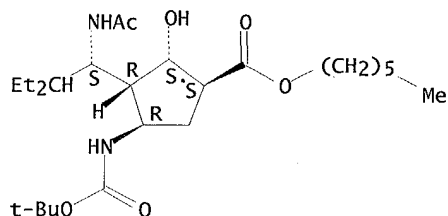
PAGE 1-B

CHET2

OBu-t

RN 357448-03-4 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, hexyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

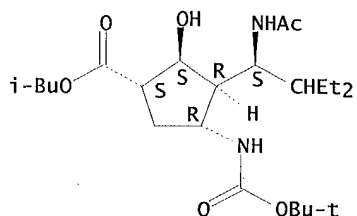
Absolute stereochemistry. Rotation (-).



RN 357448-07-8 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, 2-methylpropyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

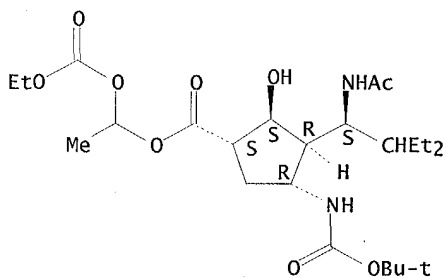
Absolute stereochemistry. Rotation (-).



RN 357448-11-4 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, 1-[(ethoxycarbonyl)oxy]ethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

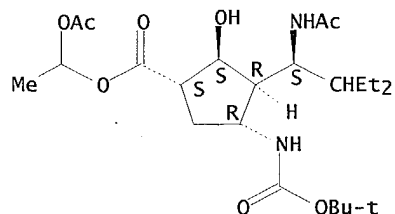
Absolute stereochemistry.



RN 357448-15-8 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, 1-(acetyloxy)ethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

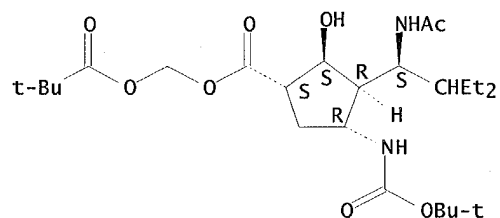
Absolute stereochemistry.



RN 357448-19-2 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetamido)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, (2,2-dimethyl-1-oxopropoxy)methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

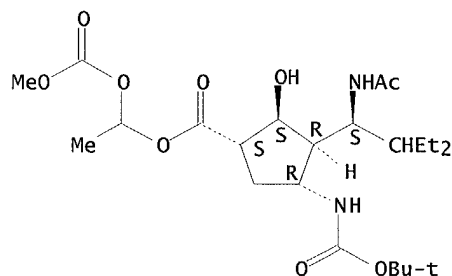
Absolute stereochemistry. Rotation (-).



RN 357448-23-8 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetamido)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, 1-[(methoxycarbonyl)oxy]ethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

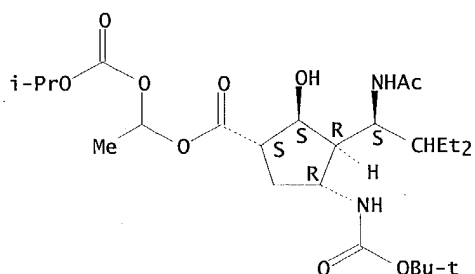
Absolute stereochemistry.



RN 357448-27-2 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetamido)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, 1-[[[(1-methylethoxy)carbonyl]oxy]ethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



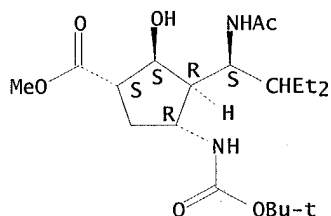
IT 229614-05-5 229614-07-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; synthesis of guanidino-cyclopentyl-carboxy derivs.
(prodrugs) as neuraminidase inhibitors)

RN 229614-05-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

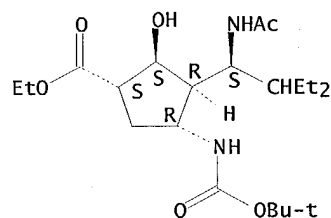
Absolute stereochemistry. Rotation (-).



RN 229614-07-7 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:460384 CAPLUS

DOCUMENT NUMBER: 131:87678

TITLE: Preparation of substituted cyclopentane and
cyclopentene compounds as neuraminidase inhibitors

INVENTOR(S): Babu, Yarlagadda S.; Chand, Pooran; Montgomery, John
A.

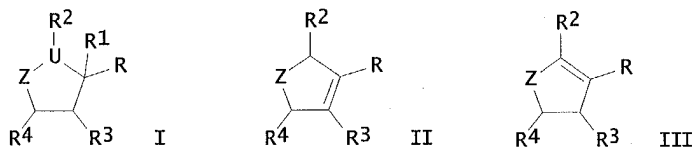
PATENT ASSIGNEE(S): Biocryst Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 196 pp.

DOCUMENT TYPE: CODEN: PIXXD2
 LANGUAGE: Patent
 FAMILY ACC. NUM. COUNT: 1 English
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933781	A1	19990708	WO 1998-US26871	19981217
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2315262	AA	19990708	CA 1998-2315262	19981217
AU 9922001	A1	19990719	AU 1999-22001	19981217
ZA 9811595	A	20000619	ZA 1998-11595	19981217
EP 1040094	A1	20001004	EP 1998-966003	19981217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9813480	A	20001010	BR 1998-13480	19981217
JP 2001527058	T2	20011225	JP 2000-526468	19981217
US 6562861	B1	20030513	US 2000-555131	20000525
NO 2000003084	A	20000814	NO 2000-3084	20000615
PRIORITY APPLN. INFO.:				
			US 1997-69956P	P 19971217
			US 1998-85252P	P 19980513
			WO 1998-US26871	W 19981217

OTHER SOURCE(S): MARPAT 131:87678
 GI

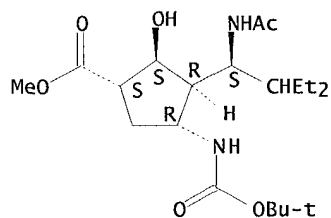


AB Title compds. I-III wherein U is CH, O, or S; Z is mono- or di-substituted carbon; R is (CH₂)_nCO₂H, (CH₂)_nSO₃H, (CH₂)_nPO₃H₂, (CH₂)_nNO₂, CH(SCH₃)₃, esters; R₁ is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl; R₂ is O; n is 0-4; R₃ is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl, haloalkyl; R₄ is (CH₂)_nOH, (CH₂)_nNH₂, substituted alkyl were prepd. as neuraminidase inhibitors. Thus, (1R,3R,4R,1'S)-(1'-acetylamino-2'-ethyl)butyl-4-(aminoimino)methylaminocyclopentan-1-carboxylic acid was prepd. and tested in vitro as neuraminidase inhibitor (IC₅₀ < 1 .mu.M).

IT 229614-05-5P 229614-06-6P 229614-07-7P
 229614-08-8P 229614-09-9P 229614-10-2P
 229614-11-3P 229614-12-4P 229614-13-5P
 229614-14-6P 229614-15-7P 229614-16-8P
 229614-61-3P 229614-62-4P 229614-63-5P
 229614-64-6P 229614-65-7P 229614-97-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of substituted cyclopentane and cyclopentene compds. as neuraminidase inhibitors)

RN 229614-05-5 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy]carbonyl]amino]-2-hydroxy-, methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

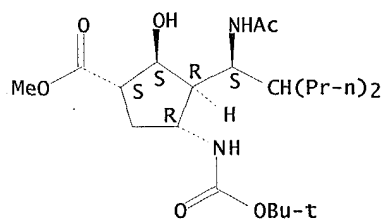
Absolute stereochemistry. Rotation (-).



RN 229614-06-6 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-propylpentyl]-4-
[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

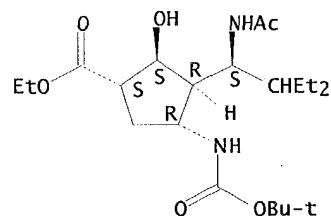
Absolute stereochemistry. Rotation (-).



RN 229614-07-7 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

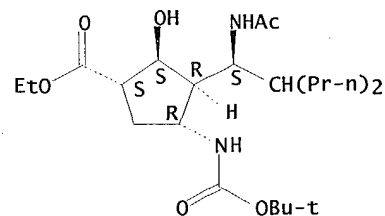
Absolute stereochemistry. Rotation (-).



RN 229614-08-8 CAPLUS

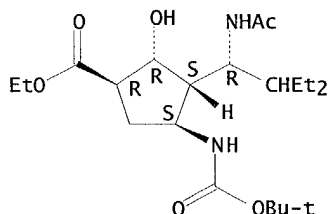
CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-propylpentyl]-4-
[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



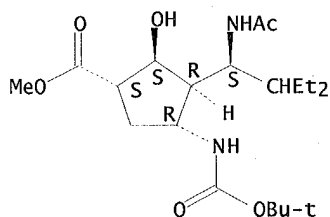
RN 229614-09-9 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-
 [[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
 (1R,2R,3S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



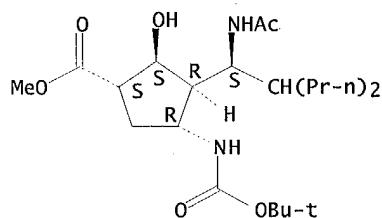
RN 229614-10-2 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-
 [[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester,
 (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



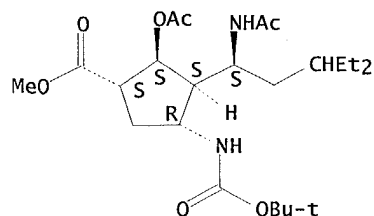
RN 229614-11-3 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-propylpentyl]-4-
 [[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, methyl ester,
 (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 229614-12-4 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-3-ethylpentyl]-2-
 (acetyloxy)-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester,
 (1R,2R,3R,4S)-rel- (9CI) (CA INDEX NAME)

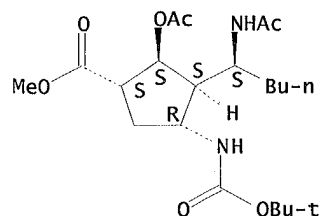
Relative stereochemistry.



RN 229614-13-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)pentyl]-2-(acetyloxy)-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1R,2R,3R,4S)-rel- (9CI) (CA INDEX NAME)

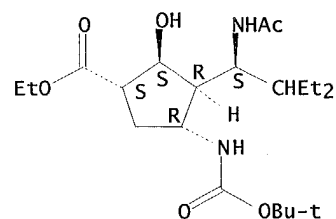
Relative stereochemistry.



RN 229614-14-6 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester, (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

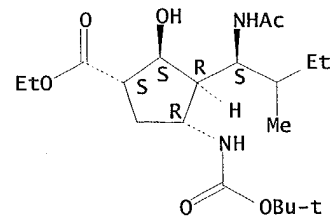
Relative stereochemistry.



RN 229614-15-7 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-methylbutyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester, (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

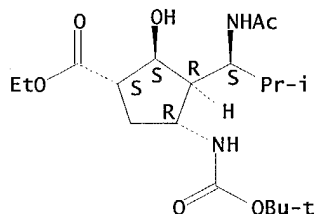
Relative stereochemistry.



RN 229614-16-8 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-methylpropyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-2-hydroxy-, ethyl ester,
(1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

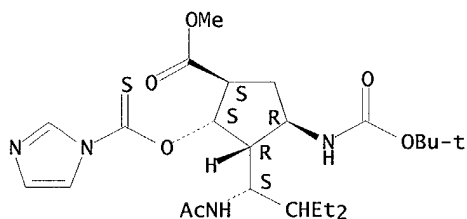
Relative stereochemistry.



RN 229614-61-3 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-2-(1H-imidazol-1-ylthioxomethoxy)-,
methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

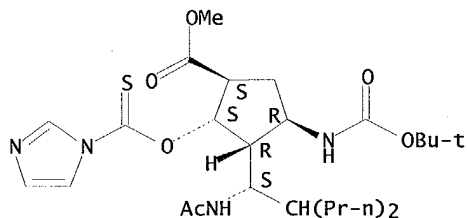
Absolute stereochemistry. Rotation (-).



RN 229614-62-4 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-propylpentyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-2-(1H-imidazol-1-ylthioxomethoxy)-,
methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

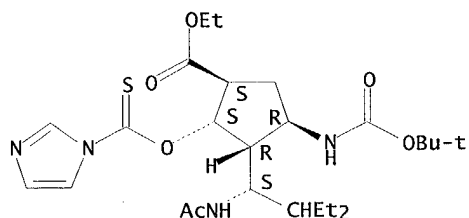
Absolute stereochemistry. Rotation (-).



RN 229614-63-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-2-(1H-imidazol-1-ylthioxomethoxy)-,
ethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

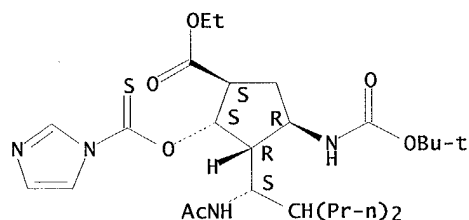
Absolute stereochemistry. Rotation (-).



RN 229614-64-6 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-propylpentyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-(1H-imidazol-1-ylthioxomethoxy)-, ethyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

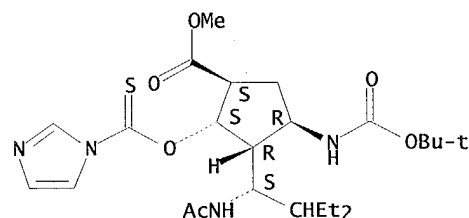
Absolute stereochemistry. Rotation (-).



RN 229614-65-7 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-(1H-imidazol-1-ylthioxomethoxy)-, methyl ester, (1R,2R,3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

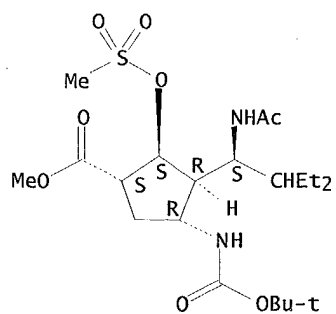


RN 229614-97-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-[[[1,1-dimethylethoxy)carbonyl]amino]-2-[(methylsulfonyl)oxy]-, methyl ester, (1S,2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

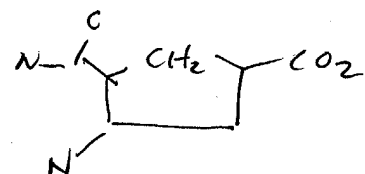
SOLOLA 10/019,217



REFERENCE COUNT:

8

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

preparation of 

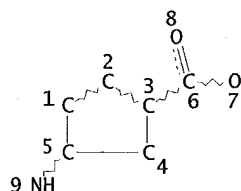
SOLOLA 10/019,217

=> D QUE L57
L13

STR

parent str

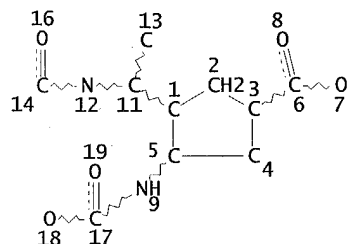
from anything



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L15 1511 SEA FILE=REGISTRY SSS FUL L13
L54 STR



la A=H

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L55 22 SEA FILE=REGISTRY SUB=L15 SSS FUL L54
L56 4 SEA FILE=CAPLUS ABB=ON PLU=ON L55
L57 4 SEA FILE=CAPLUS ABB=ON PLU=ON L56(L)PREP/RL

4 cites

=> d ibib abs hitstr L57 1-4

L57 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:787187 CAPLUS

DOCUMENT NUMBER: 136:69605

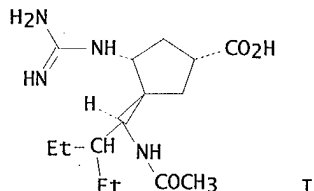
TITLE: Systematic Structure-Based Design and Stereoselective Synthesis of Novel Multi-Substituted Cyclopentane Derivatives with Potent Anti-influenza Activity
AUTHOR(S): Chand, Pooran; Kotian, Pravin L.; Dehghani, Ali; El-Kattan, Yahya; Lin, Tsu-Hsing; Hutchison, Tracy L.; Babu, Y. Sudhakar; Bantia, Shanta; Elliott, Arthur J.; Montgomery, John A.

CORPORATE SOURCE: BioCryst Pharmaceuticals Inc., Birmingham, AL, 35244, USA

SOURCE: Journal of Medicinal Chemistry (2001), 44(25), 4379-4392

PUBLISHER: CODEN: JMCMAR; ISSN: 0022-2623
American Chemical Society

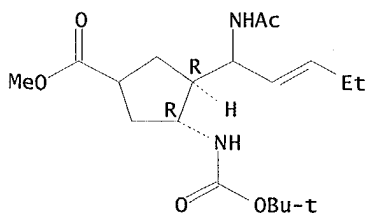
DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The design and synthesis of novel, orally active, potent, and selective inhibitors of influenza neuraminidase differing structurally from existing neuraminidase inhibitors are described. X-ray crystal structures of complexes of neuraminidase with known five- and six-membered ring inhibitors revealed that potent inhibition of the enzyme is detd. by the relative positions of the interacting inhibitor substituents (carboxylate, glycerol, acetamido, hydroxyl) rather than by the abs. position of the central ring. This led us to design potential neuraminidase inhibitors in which the cyclopentane ring served as a scaffold for substituents (carboxylate, guanidino, acetamido, alkyl) that would interact with the four binding pockets of the neuraminidase active site at least as effectively as those of the established six-membered ring inhibitors such as DANA, zanamivir, and oseltamivir. A mixt. of the isomers was prepd. initially. Protein crystallog. of inhibitor-enzyme complexes was used to screen mixts. of isomers in order to identify the most active stereoisomer. A synthetic route to the identified candidate cyclopentane I was developed, which featured (3+2) cycloaddn. of 2-ethylbutyronitrile oxide to Me (1S,4R)-4[(tert-butoxycarbonyl)amino]cyclopent-2-ene-1-carboxylate. Structures of the synthetic compds. were verified by NMR spectroscopy using nuclear Overhauser effect methodol. No new neuraminidase inhibitors discovered in this work, I has IC50 values vs neuraminidase from influenza A and B of <1 nM. These IC50 values are comparable or superior to those for zanamivir and oseltamivir, agents recently approved by the FDA for treatment of influenza.

IT 201001-80-1P 229614-66-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (systematic structure-based design and stereoselective synthesis of novel multi-substituted cyclopentane derivs. with potent anti-influenza activity)
 RN 201001-80-1 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[1-(acetilamino)-2-pentenyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry unknown.

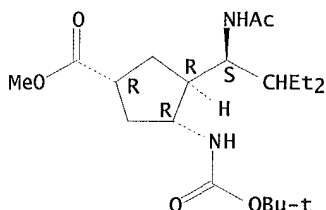


RN 229614-66-8 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetilamino)-2-ethylbutyl]-4-

SOLOLA 10/019,217

[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1R,3R,4R)- (9CI)
(CA INDEX NAME)

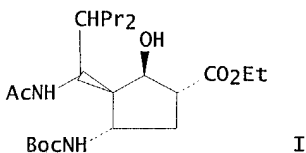
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:12400 CAPLUS
DOCUMENT NUMBER: 134:85973
TITLE: Preparation of substituted cyclopentane and cyclopentene compounds and certain intermediates
INVENTOR(S): Chand, Pooran; Elliott, Arthur J.
PATENT ASSIGNEE(S): Biocryst Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000558	A1	20010104	WO 2000-US17685	20000628
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1189862	A1	20020327	EP 2000-946871	20000628
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRIORITY APPLN. INFO.:		US 1999-140840P P 19990628 WO 2000-US17685 W 20000628		
OTHER SOURCE(S):		MARPAT 134:85973		
GI				



AB Cyclopentanes such as I were prepd. from cyclopentane-fused isoxazolines, which were obtained by reaction of nitrile oxides with cyclopentenenes. Thus, a mixt. of 15 g Et c-4-[(tert-butoxycarbonyl)amino]-t-3-(2-propylbutyl)-4,5,6,6a-tetrahydro-2aH-cyclopent[d]isoxazole-6-r-carboxylate

(II) in 120 mL EtOH/water/HOAc (1:1:1) contg. 1.5 g PtO₂ was hydrogenated at 45 psi for 60 h to give 19 g (-)-t-3-(1-amino-2-propylpentyl)-c-4-[(tert-butoxycarbonyl)amino]-t-2-hydroxycyclopentane-r-1-carboxylate, which was acetylated by Ac₂O in CH₂Cl₂ to give a 61% yield of I. The prepn. of II from 1-nitro-2-propylpentane, (-)-Et 4-[(tert-butoxycarbonyl)amino]cyclopentene-1-carboxylate, and PhNCO was described. The products were intended as neuraminidase inhibitors.

IT 316147-78-1P

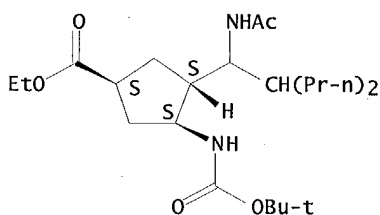
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(cyclopentanecarboxylate derivs. as neuraminidase inhibitors)

RN 316147-78-1 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[1-(acetyl amino)-2-propylpentyl]-4-[[1,1-dimethylethoxy)carbonyl]amino]-, ethyl ester, (1R,3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:460384 CAPLUS

DOCUMENT NUMBER: 131:87678

TITLE: Preparation of substituted cyclopentane and cyclopentene compounds as neuraminidase inhibitors

INVENTOR(S): Babu, Yarlagadda S.; Chand, Pooran; Montgomery, John A.

PATENT ASSIGNEE(S): Biocryst Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 196 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

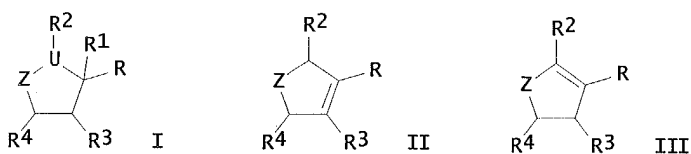
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933781	A1	19990708	WO 1998-US26871	19981217
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2315262	AA	19990708	CA 1998-2315262	19981217
AU 9922001	A1	19990719	AU 1999-22001	19981217
ZA 9811595	A	20000619	ZA 1998-11595	19981217
EP 1040094	A1	20001004	EP 1998-966003	19981217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9813480	A	20001010	BR 1998-13480	19981217
JP 2001527058	T2	20011225	JP 2000-526468	19981217

SOLOLA 10/019,217

US 6562861 B1 20030513 US 2000-555131 20000525
NO 2000003084 A 20000814 NO 2000-3084 20000615
PRIORITY APPLN. INFO.: US 1997-69956P P 19971217
US 1998-85252P P 19980513
WO 1998-US26871 W 19981217
OTHER SOURCE(S): MARPAT 131:87678
GI



AB Title compds. I-III wherein U is CH, O, or S; Z is mono- or di-substituted carbon; R is (CH₂)_nCO₂H, (CH₂)_nSO₃H, (CH₂)_nPO₃H₂, (CH₂)_nNO₂, CH(SCH₃)₃, esters; R₁ is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl; R₂ is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl, haloalkyl; R₃ is H, hydroxyalkyl, aminoalkyl, alkoxyalkyl, haloalkyl; R₄ is (CH₂)_nOH, (CH₂)_nNH₂, substituted alkyl were prepd. as neuraminidase inhibitors. Thus, (1R,3R,4R,1'S)-(-)-(1'-acetylamino-2'-ethyl)butyl-4-(aminoimino)methylaminocyclopentan-1-carboxylic acid was prepd. and tested in vitro as neuraminidase inhibitor (IC₅₀ < 1 .mu.M).

IT 229612-95-7P 229613-02-9P 229613-06-3P
229613-15-4P 229613-16-5P 229614-66-8P
229614-67-9P 229614-68-0P 229614-69-1P
229614-70-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

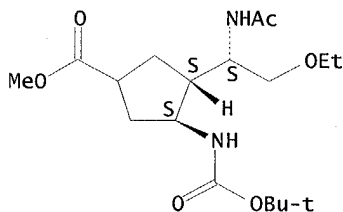
(Preparation); RACT (Reactant or reagent)

(prepn. of substituted cyclopentane and cyclopentene compds. as neuraminidase inhibitors)

RN 229612-95-7 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-ethoxyethyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (3R,4R)-rel- (9CI)
(CA INDEX NAME)

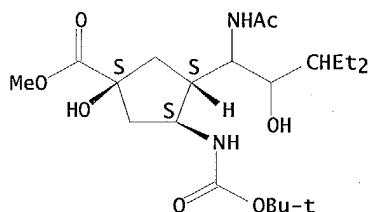
Relative stereochemistry.



RN 229613-02-9 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[1-(acetylamino)-3-ethyl-2-hydroxypentyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-hydroxy-, methyl ester, (1R,3R,4R)-rel- (9CI) (CA INDEX NAME)

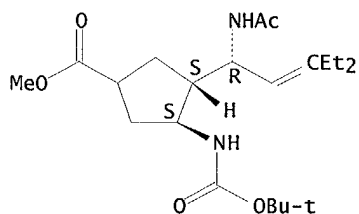
Relative stereochemistry.



RN 229613-06-3 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-3-ethyl-2-pentenyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (3S,4S)-rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.

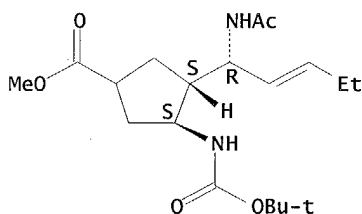


RN 229613-15-4 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-pentenyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (3S,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

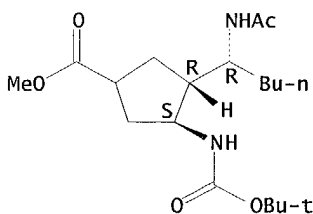
Double bond geometry unknown.



RN 229613-16-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)pentyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (3R,4S)-rel- (9CI) (CA INDEX NAME)

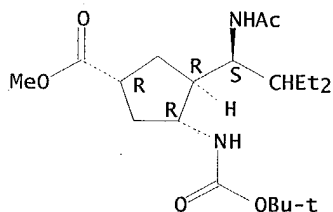
Relative stereochemistry.



RN 229614-66-8 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1R,3R,4R)- (9CI)
(CA INDEX NAME)

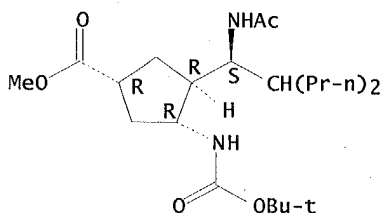
Absolute stereochemistry. Rotation (-).



RN 229614-67-9 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-propylpentyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1R,3R,4R)- (9CI)
(CA INDEX NAME)

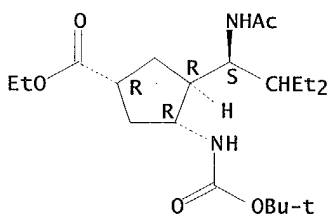
Absolute stereochemistry. Rotation (-).



RN 229614-68-0 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-ethylbutyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-, ethyl ester, (1R,3R,4R)- (9CI)
(CA INDEX NAME)

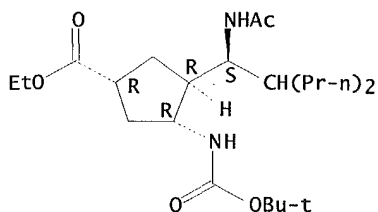
Absolute stereochemistry. Rotation (-).



RN 229614-69-1 CAPLUS

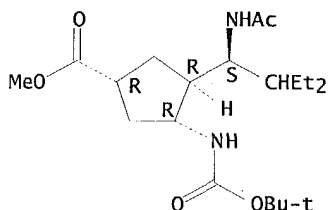
CN Cyclopentanecarboxylic acid, 3-[(1S)-1-(acetylamino)-2-propylpentyl]-4-
[[[1,1-dimethylethoxy)carbonyl]amino]-, ethyl ester, (1R,3R,4R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



RN 229614-70-4 CAPLUS
 CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetlamino)-2-ethylbutyl]-4-
 [[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (1S,3S,4S)-rel-
 (9CI) (CA INDEX NAME)

Relative stereochemistry.



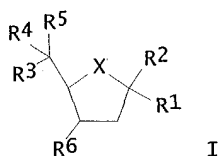
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1998:13805 CAPLUS
 DOCUMENT NUMBER: 128:101850
 TITLE: Preparation of substituted cyclopentanes as influenza
 virus neuraminidase inhibitors
 INVENTOR(S): Babu, Yarlagadda S.; Chand, Pooran; Montgomery, John
 A.
 PATENT ASSIGNEE(S): Biocryst Pharmaceuticals, Inc., USA; Babu, Yarlagadda
 S.; Chand, Pooran; Montgomery, John A.
 SOURCE: PCT Int. Appl., 206 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9747194	A1	19971218	WO 1997-US9309	19970613
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2258217	AA	19971218	CA 1997-2258217	19970613
AU 9734750	A1	19980107	AU 1997-34750	19970613
AU 723360	B2	20000824		
EP 933993	A1	19990811	EP 1997-931014	19970613
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CN 1227466	A	19990901	CN 1997-197248	19970613

SOLOLA 10/019,217

JP 2000505088	T2	20000425	JP 1998-501649	19970613
NZ 333437	A	20000526	NZ 1997-333437	19970613
BR 9711095	A	20010717	BR 1997-11095	19970613
NO 9805821	A	19990210	NO 1998-5821	19981211
KR 2000016669	A	20000325	KR 1998-710269	19981214
US 6410594	B1	20020625	US 1999-202351	19990609
PRIORITY APPLN. INFO.:			US 1996-19930P	P 19960614
			US 1997-44010P	P 19970502
			WO 1997-US9309	W 19970613
OTHER SOURCE(S):	MARPAT 128:101850			
GI				



AB Title compds. I (X = O, S, CH₂; R₁ = H, OH, NH₂, alkoxy; R₂ = H, CO₂H, SO₃H, PO₃H₂, NO₂, ester; R₃, R₄ = independently H, ester, ether, aminoalkyl, amide, alkyl; R₅ = H, NHCOR₇, NHCSR₇, NHSO₂R₇, CONHR₇, SO₂NHR₇, CH₂SO₂R₇; R₆ = H, hydroxyalkyl, aminoalkyl, cyanoalkyl, azidoalkyl; R₇ = H, alkyl, cycloalkyl, CF₃) were prepd. as influenza virus neuraminidase inhibitors. Compds. I are influenza virus neuraminidase inhibitors and can be used in treating patients infected with influenza virus. Thus, compds. I [R₁ = R₃ = R₄ = H, R₂ = CO₂H; R₅ = NHAc; R₆ = NHC(NH)NH₂] was prepd. and its inhibition of influenza virus neuraminidase (IC₅₀ = 115 .mu.M) is reported, other derivs. inhibition IC₅₀ ranged from 0.041 to 3800 .mu.M.

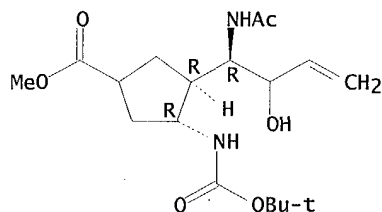
IT 201000-79-5P 201000-81-9P 201001-13-0P
201001-20-9P 201001-21-0P 201001-80-1P
201338-11-6P 201338-14-9P 201338-15-0P
201338-17-2P 201338-18-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of substituted cyclopentanes as influenza virus neuraminidase inhibitors)

RN 201000-79-5 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[1-(acetylamino)-2-hydroxy-3-butenyl]-4-[[1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, [3R(1R),4R]-rel-[partial]- (9CI) (CA INDEX NAME)

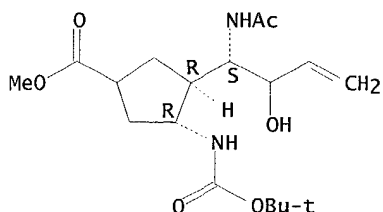
Relative stereochemistry.



RN 201000-81-9 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetylamino)-2-hydroxy-3-butenyl]-4-[[1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (3S,4S)-rel- (9CI) (CA INDEX NAME)

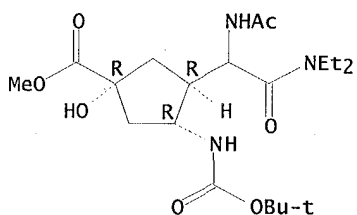
Relative stereochemistry.



RN 201001-13-0 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[1-(acetamino)-2-(diethylamino)-2-oxoethyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-hydroxy-, methyl ester, (1.alpha.,3.beta.,4.alpha.)-[partial]- (9CI) (CA INDEX NAME)

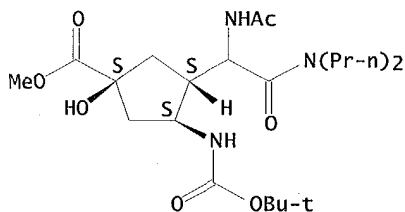
Relative stereochemistry.



RN 201001-20-9 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[1-(acetamino)-2-(dipropylamino)-2-oxoethyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-hydroxy-, methyl ester, (1.alpha.,3.beta.,4.alpha.)-[partial]- (9CI) (CA INDEX NAME)

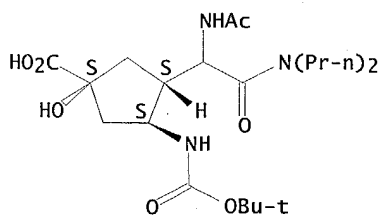
Relative stereochemistry.



RN 201001-21-0 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[1-(acetamino)-2-(dipropylamino)-2-oxoethyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-1-hydroxy-, (1.alpha.,3.beta.,4.alpha.)-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



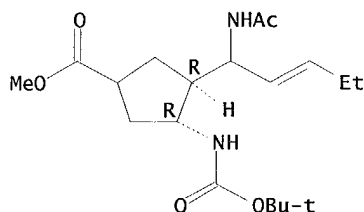
RN 201001-80-1 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[1-(acetamino)-2-pentenyl]-4-[[[(1,1-

SOLOLA 10/019,217

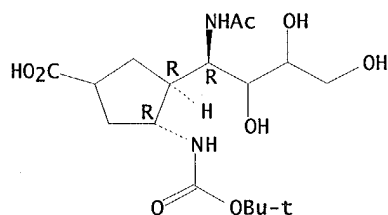
dimethylethoxy)carbonyl]amino]-, methyl ester, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



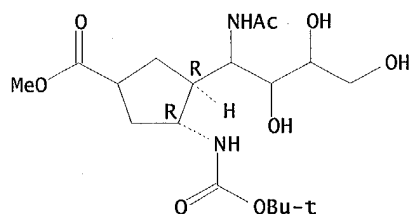
RN 201338-11-6 CAPLUS
CN Cyclopentanecarboxylic acid, 3-[1-(acetamino)-2,3,4-trihydroxybutyl]-4-
[[1,1-dimethylethoxy)carbonyl]amino]-, [3R(1R),4R]-rel-[partial]- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



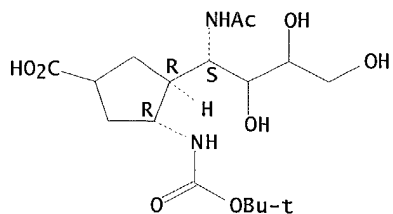
RN 201338-14-9 CAPLUS
CN Cyclopentanecarboxylic acid, 3-[1-(acetamino)-2,3,4-trihydroxybutyl]-4-
[[1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (3R,4R)-rel-
[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 201338-15-0 CAPLUS
CN Cyclopentanecarboxylic acid, 3-[(1R)-1-(acetamino)-2,3,4-
trihydroxybutyl]-4-[[1,1-dimethylethoxy)carbonyl]amino]-, (3S,4S)-rel-
(9CI) (CA INDEX NAME)

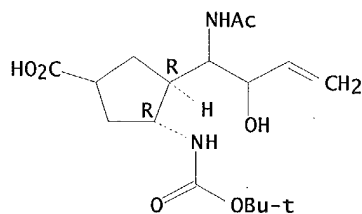
Relative stereochemistry.



RN 201338-17-2 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[1-(acetylamino)-2-hydroxy-3-butenyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, (3R,4R)-rel-[partial]- (9CI) (CA INDEX NAME)

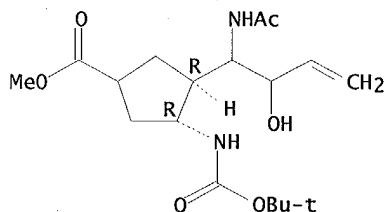
Relative stereochemistry.



RN 201338-18-3 CAPLUS

CN Cyclopentanecarboxylic acid, 3-[1-(acetylamino)-2-hydroxy-3-butenyl]-4-[[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (3R,4R)-rel-[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

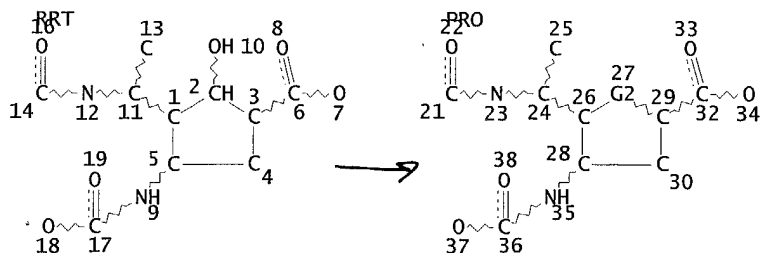


CASReact

SOLOLA 10/019,217

=> D QUE L50
L48

STR



O @20

C~H @39 40
CH~G1 @41 42

VAR G1=F/NH/20

VAR G2=41/39

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 20

CONNECT IS E2 RC AT 39

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 40

STEREO ATTRIBUTES: NONE

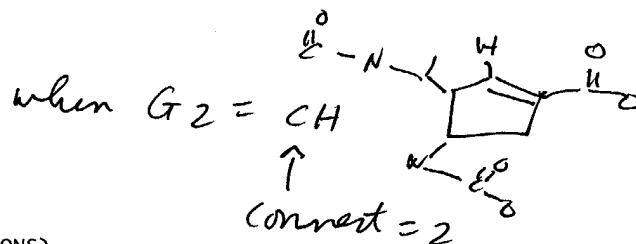
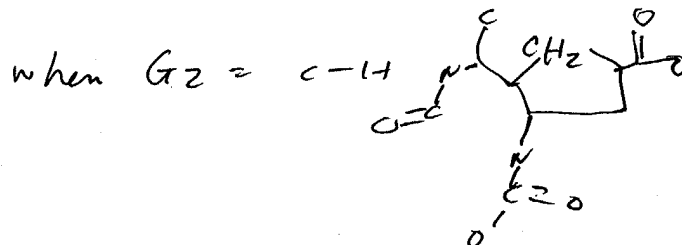
L50

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0 REACTIONS)

no cites

for the product

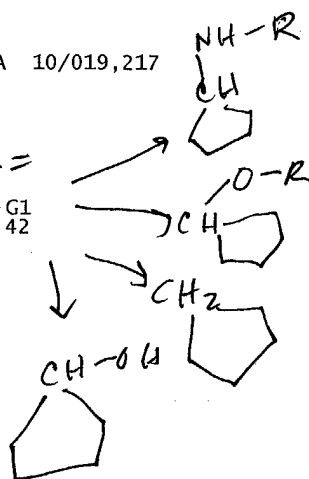
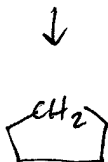
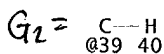
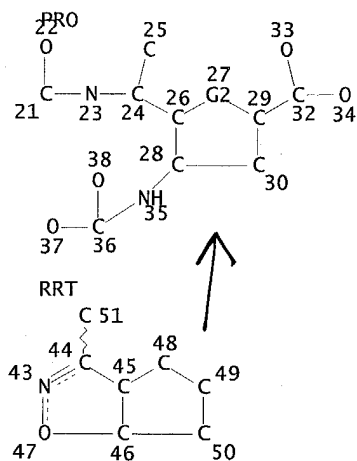


Cas react

SOLOLA 10/019,217

=> D QUE L53
L52

STR



VAR G1=H/F/NH/O

VAR G2=41/39

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 39

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

L53

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0 REACTIONS)

no cites